# Calculation of hydrogen solubility in molten alloys

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**Abstract:** A thermodynamic model was developed to calculate the hydrogen solubility in molten alloys based on the hydrogen solubility in constitutional pure liquid metals and their interaction parameters. The calculated results have a good agreement with the documented experimental results. The closer the molten alloy to an ideal liquid is, the more accurate the calculated results are. The compound forming ability and molar mixing heat of the constitutional elements take important roles in influencing the hydrogen solubility in molten alloys.

**Key words:** hydrogen solubility; molten alloy; interaction parameter

## 1 Introduction

Hydrogen can be absorbed and solved in most molten alloys, which usually leads to defects in solidified alloys as porosity, property reduction structure (e.g. hydrogen brittleness) etc[1−2]. So, the task of metallurgical engineers is always to eliminate the hydrogen content in metals. But recently, the high solubility of hydrogen in metals is being used positively to produce a new ordered porous material called GASAR which has distinct properties and wide potential applications in various fields[3−5]. The solubility of hydrogen in molten alloys is becoming more and more interested. However, the experimentally measured results of hydrogen solubility in molten alloys are not so abundant for the new usage. The reason for this situation is mainly because 1) the absolute amount of hydrogen in alloys is very low and the melting temperature of alloys is usually high, both of them lead to the difficulty in accurate measurements; 2) there are so many alloy systems that it is almost impossible to measure hydrogen solubility in various alloys one by one[6]. At the same time, there exists great scatter of experimental results in a given alloy system measured by different authors and methods[6−7]. Therefore, developing calculating models of hydrogen solubility in molten alloys is of a great

necessity.

Among various researches, Wagner's model[8] based on the interaction parameter between hydrogen and alloying elements was widely accepted for predicting hydrogen solubility in molten alloys[2, 9−11]. However, to use Wagner's model to an alloy system, the interaction parameters should be experimentally determined first. And it should be assumed that the effect of every alloying element on hydrogen solubility is independent of the addition of other alloying elements. So, Wagner's model is hard to deal with molten alloys which cannot be regarded as dilute melt and/or alloys with multi-components.

In an early research of JIANG et al[12], a theoretical model for calculating hydrogen solubility in molten aluminum alloys had been developed based on hydrogen solubility in pure metals and thermodynamic properties of molten alloys which are expressed by approximate models. In the present study, the theoretical model has been developed to calculate hydrogen solubility in more multi-component alloys based on more precise experimental values of thermodynamic properties. With this model, hydrogen solubility in binary alloys which can be regarded as dilute melt and ternary alloys can all be calculated. For convenience of comparing with documented experimental results, hydrogen pressure is set at 0.1 MPa.

## 2 Theoretical model

Commonly, hydrogen solubility $C_H(10^{-2}$ mL/g) in molten alloys under normal pressure is ruled by Sieverts' law[1, 8]:

$$C_H = \sqrt{p_{H_2}/p_0}\exp[-\Delta G_m^{\Theta}/(RT)] \qquad (1)$$

where $G_m^{\Theta}$ (J/mol) is the change of molar free energy of hydrogen during solution; $p_{H_2}$(Pa) is the pressure of hydrogen on the molten alloy; $p_0$ is the standard pressure and is usually set to be 0.1 MPa; $R$ is molar gas constant, 8.314 J/(mol·K$^{-1}$); $T$(K) is the temperature of the molten alloy.

For an alloy melt which can be regarded as ideal liquid, $\Delta G_m^{\Theta}$ could be expressed as

$$\Delta G_m^{\Theta} = \sum x_i \Delta G_i^{\Theta} \qquad (2)$$

where $x_i$ is the mole fraction of component $i$; $\Delta G_i^{\Theta}$ (J/mol)is the change of molar free energy of hydrogen in pure molten element $i$. For alloy melts near to the ideal liquid, Eq.(2) could be modified to[2, 13]

$$\Delta G_m^{\Theta} = \sum x_i \Delta G_i^{\Theta} - \Delta G_m^{ex} \qquad (3)$$

where $\Delta G_m^{ex}$(J/mol) is the excess molar free energy. By solving Eq.(1) and Eq.(3), $C_H$ can be expressed as

$$\ln C_H = \sum x_i \ln C_{H,i} + \Delta G_m^{ex}/(RT) \qquad (4)$$

where $C_{H,i}$ ($10^{-2}$ mL/g) is the hydrogen solubility in liquid component $i$ at temperature $T$.

The excess molar free energy of liquid alloys could either be calculated by various models[14−16] or experimentally measured[17−18], where the former ones are more precise than the later ones. For a binary alloy, the experimental values could be expressed by Redlich-Kister polynomials[19]:

$$\Delta G_m^{ex} = x_i x_j L_{i,j} \qquad (5)$$

where $L_{i,j}$ (J/mol)is a binary parameter describing the interaction between components $i$ and $j$, as follows:

$$L_{i,j} = \sum_{n=0}^{N} {}^n L_{i,j}(x_i - x_j)^n \qquad (6)$$

For a ternary alloy melt $i$-$j$-$k$, the excess molar free energy of the alloy system $\Delta G_m^{ex}$ could be described as follows:

$$\Delta G_m^{ex} = x_i x_j L_{i,j} + x_j x_k L_{j,k} + x_k x_i L_{k,i} + x_i x_j x_k L_{i,j,k} \qquad (7)$$

where $L_{i,j,k}$ (J/mol)is a ternary interaction parameter.

## 3 Results

For convenience of comparing with experimental results, six binary alloys with low alloying content which

form terminal solid solution during solidification (Al-2.5Mg, Al-2Li, Al-4Cu, Al-6Zn, Al-4Si, Fe-5.6Cu), six binary alloy and two ternary alloy melts with high alloying content which form isomorphic solid solution, eutectic or peritectic reaction during solidification (Fe-Ni, Fe-Cr, Co-Fe, Cu-Ni, Ni-Co, Ni-Cr, Fe-Ni-Co, Fe-Ni-Cr) are chosen for study. The parameters $L_{i,j}$ for the binary alloys and $L_{i,j,k}$ for the ternaries alloys are listed in Table 1. The hydrogen solubility in pure liquid metals are listed in Table 2.

**Table 1** Interaction parameter of molten alloys

| $L_{i,j}$, $L_{i,j,k}$/(J·mol$^{-1}$) | Literature |
|---|---|
| $L_{Al,Mg}$=−12 000+8.566$T$+(1 894−3$T$)($x_{Al}$−$x_{Mg}$)+ 2 000 ($x_{Al}$−$x_{Mg}$)$^2$ | [20] |
| $L_{Al,Zn}$=10 466−3.393$T$ | [21] |
| $L_{Al,Li}$=−12 964−5.035 5$T$+(−19 160+15.631 9$T$) ($x_{Al}$−$x_{Li}$)+(14 718−11.207 7$T$)($x_{Al}$−$x_{Li}$)$^2$ | [22] |
| $L_{Al,Cu}$=−66 622+8.1$T$+(46 800−90.8$T$+10$T$ln$T$) ($x_{Al}$− $x_{Cu}$)+−2 812($x_{Al}$−$x_{Cu}$)$^2$ | [23] |
| $L_{Al,Si}$=−11 340−1.234$T$+(−3 531+1.367$T$)($x_{Al}$−$x_{Si}$)+ 2 265($x_{Al}$−$x_{Si}$)$^2$ | [23] |
| $L_{Fe,Cu}$=36 270−2.78$T$+(8 181−5.223$T$)($x_{Fe}$−$x_{Cu}$)+ (16 635−7.434$T$)($x_{Fe}$−$x_{Cu}$)$^2$ | [24] |
| $L_{Fe,Ni}$=−16 700+4.287 5$T$+(9 000−3.7$T$)($x_{Fe}$−$x_{Ni}$)+ (−1 500+1.262 5$T$)($x_{Fe}$−$x_{Ni}$)$^2$ | [25] |
| $L_{Co,Fe}$=−9 800+8.37$T$+(−2 350−3.75$T$)($x_{Co}$−$x_{Fe}$) | [25] |
| $L_{Ni,Co}$=1 750−2.225$T$+(300+0.125$T$)($x_{Ni}$−$x_{Co}$) | [25] |
| $L_{Ni,Cr}$=−1 275−5.387$T$−2 700($x_{Ni}$−$x_{Cr}$) | [26] |
| $L_{Cu,Ni}$=−14 259+0.45$T$ | [27] |
| $L_{Fe,Cr}$=−6 500+4.90$T$+(−1 750+1.90$T$)($x_{Fe}$−$x_{Cr}$) | [28] |
| $L_{Fe,Ni,Co}$=−5 641+0.530$T$ | [25] |
| $L_{Fe,Ni,Cr}$=43 700−20.18$T$ | [28] |

**Table 2** Solubility of hydrogen in liquid pure metals

| Liquid metal | Hydrogen solubility/($10^{-2}$mL·g$^{-1}$) | Literature |
|---|---|---|
| Fe | ln$C_H$=5.482−4 009/$T$+1/2ln($p_{H_2}/p_0$) | [7] |
| Ni | ln$C_H$=5.217−2 593/$T$+1/2ln($p_{H_2}/p_0$) | [7] |
| Cu | ln$C_H$=5.623−5 354/$T$+1/2ln($p_{H_2}/p_0$) | [7] |
| Co | ln$C_H$=4.87−3 684/$T$+1/2ln($p_{H_2}/p_0$) | [1] |
| Cr | ln$C_H$=9.91−12 273/$T$+1/2ln($p_{H_2}/p_0$) | [29] |
| Al | ln$C_H$=6.247−6 159/$T$+1/2ln($p_{H_2}/p_0$) | [7] |
| Mg | ln$C_H$=6.558−2 533/$T$+1/2ln($p_{H_2}/p_0$) | [7] |
| Zn | ~0 | [2, 29] |
| Si | ln$C_H$=22.82−29 243/$T$+1/2ln($p_{H_2}/p_0$) | [29] |
| Li | ln$C_H$=16.527 6−5 208/$T$+1/2ln($p_{H_2}/p_0$) | [29] |

The hydrogen solubilities in six binary alloy melts with low alloying content increase with increasing temperature, as shown in Fig.1, which coincide with the experimental results. Furthermore, it could be found that the calculated values in Al-4Cu, Al-6Zn and Al-4Si show better agreement with experimental results than those in Al-2.5Mg, Al-2Li and Fe-5.6Cu. The hydrogen solubility
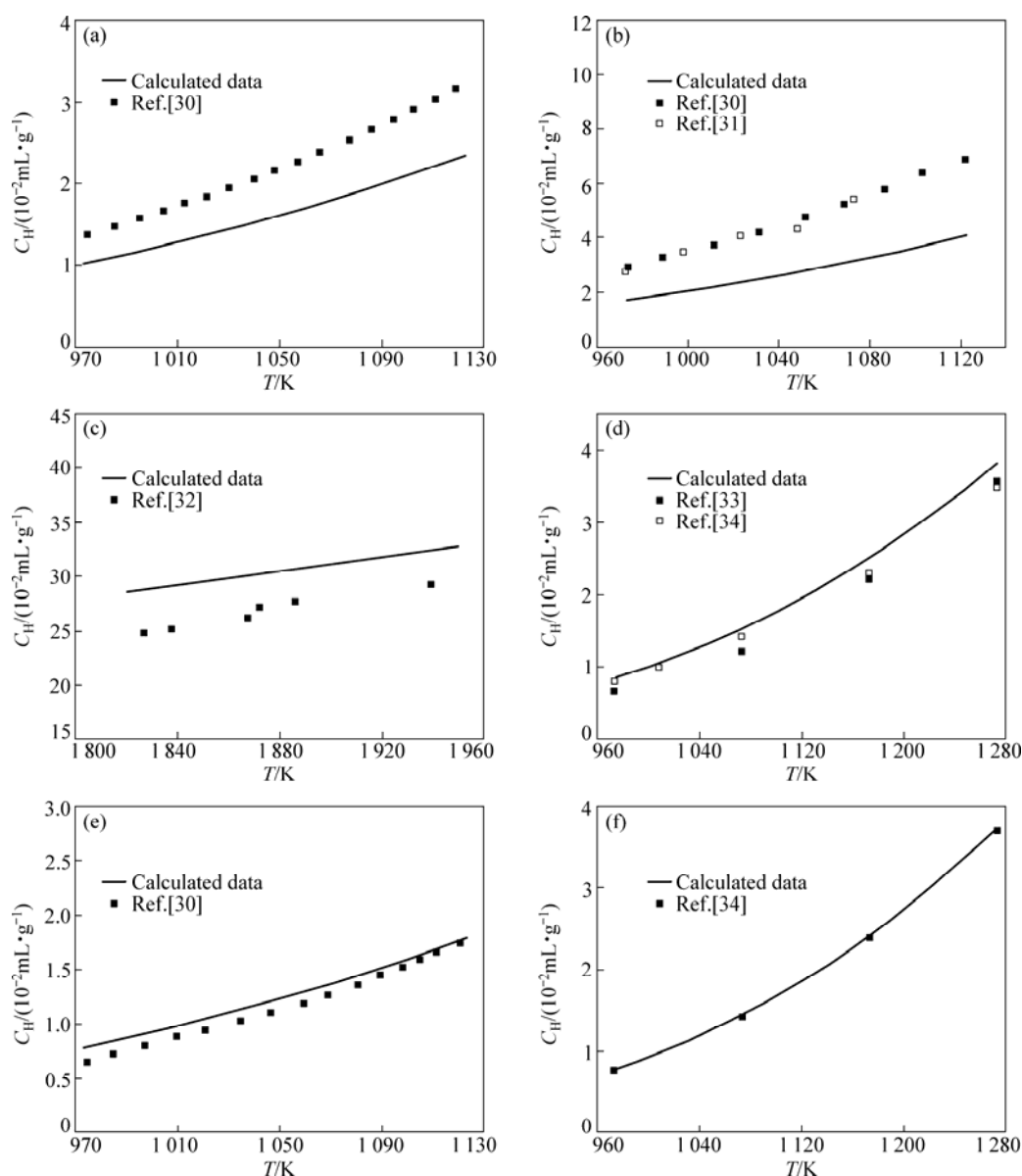
**Fig.1** Hydrogen solubilities in binary alloy melts with low alloying content ($p_{H_2}$=0.1 MPa): (a) Al-2.5Mg; (b) Al-2Li; (c) Fe-5.6Cu; (d) Al-4Cu; (e) Al-6Zn; (f) Al-4Si

values in the six binary alloy melts with high alloying content are represented in Fig.2, which shows that they have a similar changing tendency over the entire investigated composition range with experimental values. There exist some large deviations in Fe-Ni, Co-Fe and Ni-Co alloys that would be discussed later. Among those ternary alloy systems, for the Fe-Ni-Cr alloy, the calculated hydrogen solubility shows good agreement with documented value along the pseudo-binary path, as shown in Fig.2(g). And for the Fe-Ni-Co alloy, the predicted hydrogen solubility shows larger deviation than in Fe-Ni-Cr system, as shown in Fig.2(h).

# 4 Discussion

By comparing the calculated hydrogen solubilities

in all fourteen alloys with the documented experimental results, it is believed that the proposed model could be used to predict hydrogen solubility in most molten alloys. There exist also some disagreements of calculated values with experimental results.

For the hydrogen solubilities in Ni-Co, Fe-Ni and Co-Fe alloys, the values documented in Ref.[40] have large deviations from others and the calculated results, as shown in Fig.2(c)−(e) with solid circles. We believe that these values are doubtable.

Generally speaking, in molten alloys of isomorphous systems (e.g. Fe-Cr), the calculated hydrogen solubility matches well with the experimental result because the molten alloy is near to an ideal solution.

For alloys with alkali and alkaline-earth elements
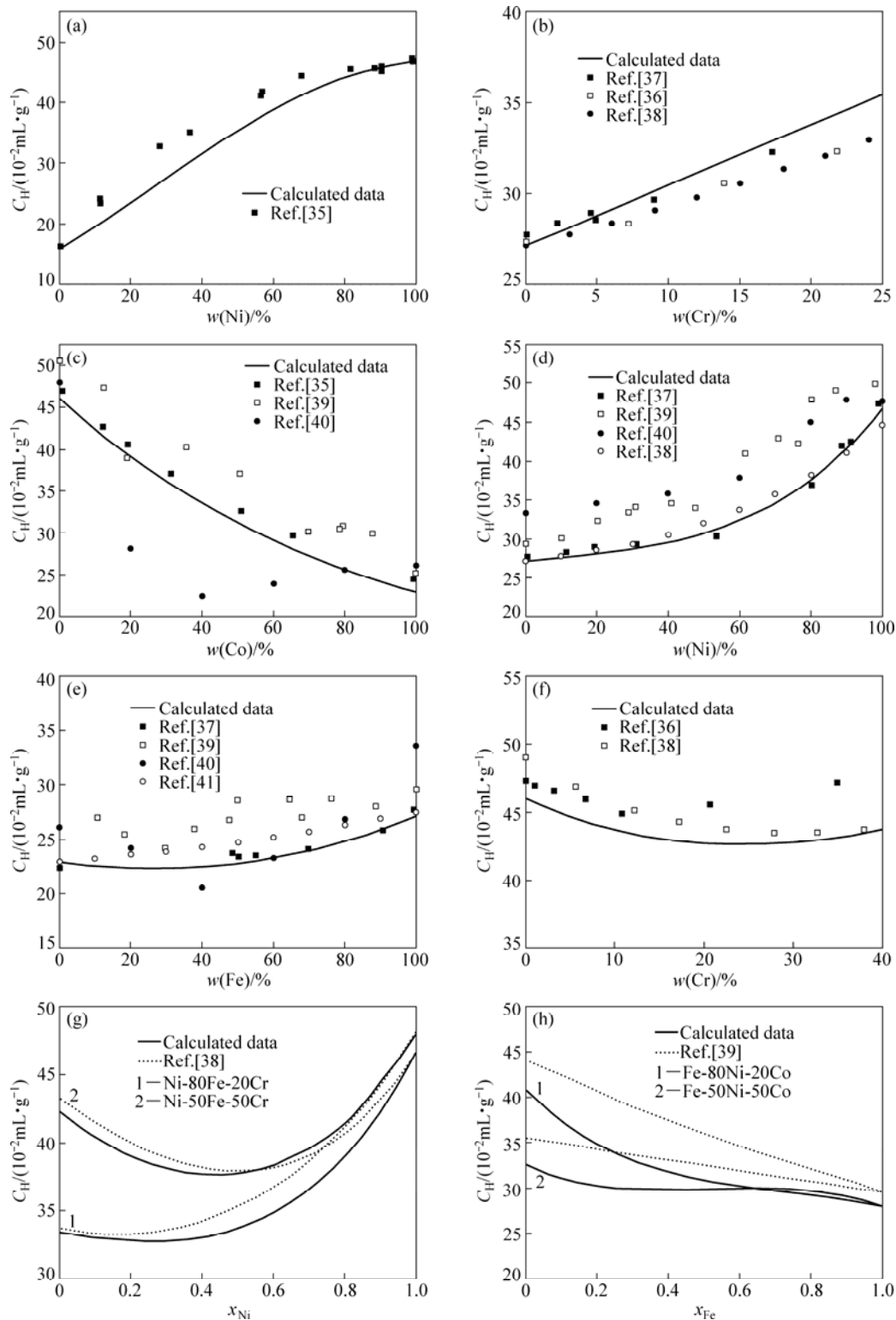
**Fig.2** Hydrogen solubilities in binary and ternary alloy melts with high alloying content at 1 873 K ($p_{H_2}$=0.1 MPa): (a) Cu-Ni; (b) Fe-Cr; (c) Ni-Co; (d) Fe-Ni; (e) Co-Fe; (f) Ni-Cr; (g) Fe-Ni-Cr; (h) Fe-Ni-Co

(e.g. Al-Li and Al-Mg), there exists relatively large difference between calculated and experimental results because alkali and alkaline-earth elements tend to form hydrides, which greatly increase the hydrogen solubility in alloys with these elements[29, 42].

　　Furthermore, in the six binary alloy systems with

high alloying content shown in Fig.2, the Ni-Cr alloy exists an eutectic point in a composition of 54%Cr (mass fraction) at 1 618 K[43], showing large difference between the calculated and experimental results. Considering the peritectic range existing in Fe-Ni and Co-Fe alloys on the iron-rich side is small[43], all the

other five alloys could be regarded as near to isomorphous systems. In an isomorphous molten alloy, the lower the molar mixing heat $\Delta H$(J/mol), the closer to an ideal solution the alloy[44−45]. The molar mixing heats of the five liquid alloys are reported in Fig.3, which are calculated by the equations shown in Table 3. It could be found that the molar mixing heats of Fe-Cr, Co-Ni and Co-Fe are much smaller than those of the other two alloys, which indicates a much smaller difference between the calculated results and the experimental results, as shown in Fig.2(b)−(e).

Additionally, various measurement errors may be contained in experimental results due to many factors[6]. The hydrogen solubility in liquid iron measured by YANG[32] is much smaller than others[1, 7], which may lead to an similar tendency in liquid Fe-5.6Cu, as shown in Fig.1(c). Similarly, considering solubilities of hydrogen in liquid Ni-Co, Fe-Ni and Co-Fe alloys published by BLOSSEY and PEHLKE[39] being higher than calculated ones, as shown in Fig.2(c)−(e) with hollow squares, it may indicate that the measured hydrogen solubility in molten Fe-Co-Ni alloy will present a negative deviation from calculated ones, as shown in Fig.2(g).
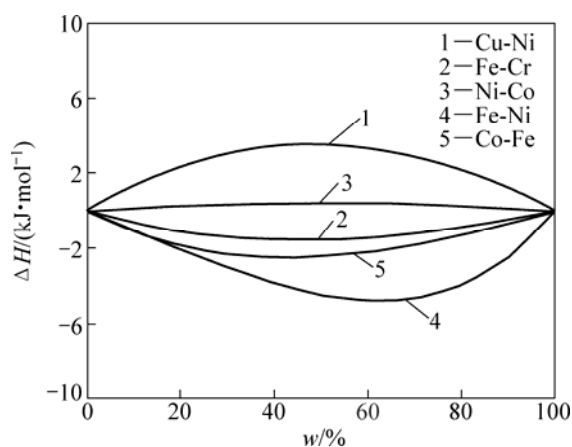


**Fig.3** Molar mixing heat of Cu-Ni, Fe-Cr, Ni-Co, Fe-Ni and Co-Fe molten alloys

**Table 3** Molar mixing heat values of Cu-Ni, Fe-Cr, Ni-Co, Fe-Ni and Co-Fe molten alloys

| Alloy | $\Delta H/(kJ \cdot mol^{-1})$ | Literature |
|---|---|---|
| Cu-Ni | $\Delta H = x_{Cu}(14.02x_{Ni} + 2.82\,x_{Ni}^2)$ | [27] |
| Fe-Cr | $\Delta H = x_{Fe}(-7.8x_{Cr} + 3.5\,x_{Cr}^2)$ | [28] |
| Ni-Co | $\Delta H = x_{Ni}(2.05x_{Co} - 0.6\,x_{Co}^2)$ | [25] |
| Fe-Ni | $\Delta H = x_{Fe}(-10.5x_{Ni} - 12\,x_{Ni}^2 - 6\,x_{Ni}^3)$ | [25] |
| Co-Fe | $\Delta H = x_{Co}(-12.15x_{Fe} + 4.7\,x_{Fe}^2)$ | [25] |

## 5 Conclusions

1) The hydrogen solubility in molten alloys can be calculated thermodynamically with the hydrogen solubility in constitutional pure liquid metals and their interaction parameters. The closer the molten alloy to an ideal liquid is, the more accurate the calculated results are.

2) Molten alloys with hydride forming elements have higher hydrogen solubilities than thermodynamically predicted results.

3) In molten alloys near to an isomorphous system, the lower the molar mixing heat, the closer the molten alloy to an ideal solution, and the higher the calculating accuracy.

## References

[1]    CHEN Yong-ding, YU Xin-chang. Hydrogen in metals and alloys [M]. Beijing: Metallurgical Industry Press, 1988: 15−107. (in Chinese)

[2]    CHERNEYA D F. Gases in nonferrous metals and alloys [M]. HUANG Liang-yu, YAN Ming-shan. Beijing: Metallurgical Industry Press, 1989: 54−82. (in Chinese)

[3]    SHAPOVALOV V I, BOYKO L.  Gasar—A new class of porous materials [J]. Advanced Engineering Materials, 2004, 6(6): 407−410.

[4]    LIU Yuan, LI Yan-xiang. A theoretical study of Gasarite eutectic growth [J]. Scripta Materialia, 2003, 49(5): 379−386.

[5]    SHAPOVALOV V I, WITHERS J C. Hydrogen technology for porous metals (Gasars) production [C]//BOGDAN B, SVETLANA Y Z, DMITRY V S, VALERLY V K, AYLER V. Carbon nanomaterials in clean energy hydrogen systems. Berlin: Springer Netherlands, 2009: 29−51.

[6]    BACCEPMAN A M, KUNIN A A, SYROVOI IU N. Measurement of the gas in metals [M]. ZHANG Zhong-hao, JIN Qin-han. Shanghai: Shanghai Science and Technology Press, 1981: 1. (in Chinese)

[7]    ZHANG Hua-wei, LI Yan-xiang, LIU Yuan. Hydrogen solubility in pure metals for Gasar process [J]. Acta Metallurgica Sinica, 2007, 43(2): 113−118. (in Chinese)

[8]    WAGNER C. Thermodynamics of alloys [M]. Cambridge: Addison-Wesley Press, 1952: 51.

[9]    LIN R Y, HOCH M. A solubility of hydrogen in molten aluminum alloys [J]. Metallurgical Transactions A, 1989, 20(9): 1785−1791.

[10]   ANYALEBECHI P N. Analysis of the effects of alloying elements on hydrogen solubility in liquid aluminum alloys [J]. Scripta Metallurgica et Materialia, 1995, 33(8): 1209−1216.

[11]   SOKOLOV V M, FEDORENKO I V. Estimation of hydrogen solubility in liquid alloys of iron, nickel and copper [J]. International Journal of Hydrogen Energy, 1996, 21(11−12): 931−934.

[12]   JIANG Guang-rui, LIU Yuan, LI Yan-xiang, GUO Jing-jie, SU Yan-qing. A model for calculating solubility of hydrogen in molten aluminum alloys [J]. Acta Metallurgica Sinica, 2007, 44(2): 129−133. (in Chinese)

[13]   O'CONNELLl J P, PRAUSNITZ J M. Thermodynamics of gas solubility in mixed solvents [J]. Industrial and Engineering Chemistry Fundamentals, 1964, 3(4): 347−351.

[14]   LUPIS C H P, ELLIOTT J F. Prediction of enthalpy and entropy interaction coefficients by the central atoms theory [J]. Acta Metallurgica, 1967, 15(2): 265−276.

[15]   CHOU K C. A general solution model for predicting ternary thermodynamic properties [J]. Calphad, 1995, 19(3): 315−325.

[16]   JIANG Guang-rui, LIU Yuan, LI Yan-xiang, GUO Jing-jie, SU Yan-qing. Improvement of calculation method for the activity

coefficient of multi-component alloys [J]. Acta Metallurgica Sinica, 2007, 43(5): 504−508. (in Chinese)

[17] SOMMER F J. Thermodynamics of liquid alloys [J]. Journal of Non-Crystalline Solids, 2007, 353(32−40): 3709−3716.

[18] WANG Hai-chuan, DONG Yuan-chi. Measurement and calculation methods of metallurgical thermodynamic data [M]. Beijing: Metallurgical Industry Press, 2005: 95−111. (in Chinese)

[19] REDLICH O, KISTER A T. Algebraic representation of thermodynamic properties and the classification of solutions [J]. Industrial & Engineering Chemistry, 1948, 40(2): 345−348.

[20] LIANG P, TARFA T, ROBINSON J A, WAGNER S, OCHIN P, HARMELIN M G, SEIFERT H J, LUKAS H L, ALDINGER F. Experimental investigation and thermodynamic calculation of the Al-Mg-Zn system [J]. Thermochimica Acta, 1998, 314(1−2): 87−110.

[21] MIETTINEN J. Thermodynamic description of the Cu-Al-Zn and Cu-Sn-Zn systems in the copper-rich corner [J]. Calphad, 2002, 26(1): 119−139.

[22] CHEN S W, JAN C H, LIN J C, CHANG Y A. Phase equilibria of the Al-Li binary system [J]. Metallurgical Transactions A, 1989, 20(11): 2247−2258.

[23] MIETTINEN J. Thermodynamic description of the Cu-Al-Si system in the copper-rich corner [J]. Calphad, 2007, 31(4): 449−456.

[24] MIETTINEN J. Thermodynamic description of the Cu-Fe-Mn system at the Cu-Fe side [J]. Calphad, 2003, 27(2): 141−145.

[25] TOMISKA J. Computer-aided thermodynamics of liquid ternary Fe-Ni-Co alloys by Knudsen cell mass spectrometry [J]. Journal of Alloys and Compounds, 2004, 373(1−2): 142−150.

[26] TOMISKA J, KOPECKY K, BELEGRATIS M S, MYERS C. Thermodynamic mixing functions and phase equilibria in the nickel-chromium system by high-temperature Knudsen cell mass spectrometry [J]. Metallurgical and Materials Transactions A, 1995, 26(2): 259−265.

[27] TURCHANIN M A. Phase equilibria and thermodynamics of binary copper systems with 3d-metals. VI. Copper-nickel system [J]. Powder Metallurgy and Metal Ceramics, 2007, 46(9−10): 467−477.

[28] TOMISKA J. The system Fe-Ni-Cr: Revision of the thermodynamic description [J]. Journal of Alloys and Compounds, 2004, 379(1−2): 176−187.

[29] MANCHESTER F D. Phase diagrams of binary hydrogen alloys [M]. Materials Park: ASM International, 2000: 1.

[30] ANYALEBECHI P N. Attempt to predict hydrogen solubility limits in liquid multicomponent aluminum alloys [J]. Scripta Materialia, 1996, 34(4): 513−517.

[31] ANYALEBECHI P N, TALBOT D E J, GRANGER D A. Solubility of hydrogen in solid binary aluminum-lithium alloys [J]. Metallurgical Transactions B, 1989, 20(4): 523−533.

[32] YANG Wei-chen. The solubility of hydrogen in liquid iron, nickel, iron-copper and iron-copper-nickel alloys [J]. Acta Metallurgica Sinica, 1964, 7(1): 1−11. (in Chinese)

[33] LIN R Y, HOCH M. A solubility of hydrogen in molten aluminum alloys [J]. Metallurgical Transactions A, 1989, 20(9): 1785−1791.

[34] LI Min. Determination of hydrogen content in aluminum and its alloys [D]. Harbin: Harbin Institute of Technology, 2006: 14−20. (in Chinese)

[35] BAGSHAW T, MITCHELLl A. Solubility of hydrogen in some liquid alloys of nickel [J]. Iron and Steel Institute Journal, 1966, 204(Part 2): 87−90.

[36] WEINSTEIN M, ELLIOTT J F. Solubility of hydrogen in liquid iron alloys [J]. Transactions of the Metallurgical Society of AIME, 1963, 227(2): 382−393.

[37] BAGSHAW T, ENGLEDOW D, MITCHELL A. Solubility of hydrogen in some liquid iron-based alloys [J]. Iron and Steel Institute Journal, 1965, 203(Part 2): 160−165.

[38] MITRA M, LANGE K W. Experimental studies on hydrogen solubility in liquid ternary iron-nickel-chromium alloys [J]. Steel Research, 1990, 61(8): 353−358.

[39] BLOSSEY R G, PEHLKE R D. Solubility of hydrogen in liquid Fe-Co-Ni alloys [J]. Metallurgical and Materials Transactions B, 1971, 2(11): 3157−3161.

[40] BUSCH T, DODD R A. Solubility of hydrogen and nitrogen in liquid alloys of iron, nickel, and cobalt [J]. Transactions of the Metallurgical Society of AIME, 1960, 218(3): 488−490.

[41] MITRA M, LANGE K W. Effect of chromium on the hydrogen solubility in liquid ternary iron-cobalt-chromium alloys [J]. Steel Research, 1988, 59(9): 394−398.

[42] HUBBERSTEY P, ADAMS P F, PULHAM R J, DOWN M G, THUNDER A E. Hydrogen in liquid alkali metals [J]. Journal of the Less-Common Metals, 1976, 49: 253−269.

[43] American Society for Metals. ASM handbook V.3. Alloy phase diagrams[M]. Materials Park: ASM International, 1992.

[44] WILSON J R. Structure of liquid metals and alloys [J]. Metallurgical Reviews, 1965, 10(40): 381−590.

[45] KUBASCHEWSKI O. The thermodynamic stability of metallic phases [C]//RUDMAN P S, STRINGER J, JAFFEE R I. Proceeding 1st Battelle Materials Science Colloquium. New York: McGraw-Hill Book Company, 1966: 63−83.

# 氢在合金熔体中的溶解度计算

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摘 要：基于氢在纯金属中的溶解度数据以及合金之间的相互作用系数，提出氢在合金熔体中溶解度的热力学计算模型。计算结果与文献中的实验数据吻合得很好。结果表明，合金熔体的性质越接近理想溶液，计算结果越准确，合金元素形成化合物的能力及其摩尔混合热对氢在合金熔体中的溶解度有重要影响。

关键词：氢溶解度；合金熔体；相互作用系数

**(Edited by YANG Hua)**